phenol, 4,4'-butylidenebis-4731-84-4 | DTXSID20280701

Model Performance

| | n . |
|--------|--------|
| Model | I)ata |
| Widdei | Data |
| | |

Weighted KNN model

| 5-fold CV (7 | 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|--------------|-----------------|------|----------------|------|------------|--|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE | |
| 0.72 | 51.8 | 0.74 | 50.3 | 0.73 | 52.7 | |

Model Results

Predicted value: 142 °C

Global applicability domain: Inside

Local applicability domain index: 9.13e-01

Confidence level: 6.49e-01

Nearest Neighbors from the Training Set

Image not found

phenol, 4,4'-butylidenebis-

Measured: 137 Predicted: 142 Image not found

Bisphenol B Measured: 121 Predicted: 140 Image not found

4,4'-Propane-1,1-diyldiphenol

Measured: 132 Predicted: 133

Image not found

Bisphenol A
Measured: 153
Predicted: 144

Image not found

meso-Hexestrol Measured: 187 Predicted: 157